Method to Determine Thermophysical Properties in Gaseous Phase Having Physical Background-Discussion on Third-Virial-Coefficient by Using Reliable Information for CO₂, Propane, and Isobutane

Yuki Kurokawa and Haruki Sato ^{c, s}
Keio University, Graduate School of Science and Technology, Yokohama, Kanagawa, Japan
hsato@sd.keio.ac.jp

Existing fundamental thermodynamic equations of state are able to represent available experimental data very precisely. On the other hand, even those equations are not reliable enough for representing properties such as the third virial coefficient in the gaseous phase. We have pointed out the difficulty in measuring accurately near the saturation state, and in determining the third virial-coefficient in the gaseous phase. Thermophysical properties such as pvT, sound speed, heat capacity, and viscosity, are fundamental data required to design turbines, compressors, and heat exchangers in various energy conversion systems such as power plants, heat pumps, and refrigerators. Recent powerful mathematical software makes it possible to determine parameters of intermolecular potential models from complicated relationships between thermophysical properties, and models including cluster or collision integrals. Using reliable thermophysical information such as very accurate fundamental equation of state and experimental data on CO2, a set of parameters for the Stockmayer potential model were derived from accurate thermodynamic property values, making it possible to calculate the third virial coefficient and predict thermophysical properties including viscosity having an uncertainties in the same range as the best experimental data in the gaseous phase. The range of input data required for determining reliable parameters, possibly yielding a reliable range of a virial equation having second and third virial-coefficients, and deviations of the experimental data from the virial equation not only for CO2 but for propane and isobutane are discussed.